Proposed Plan of Work

The present study has been designed as follows:

1. Conceptualization of novel topological descriptors based on distance, adjacency, and adjacency-cum-distance based matrices.

2. Development of computer program for calculating the values of novel topological descriptors using a high-level language.

3. Comparison of the discriminating power and degeneracy of novel descriptors with well-known distance based, adjacency based and adjacency-cum-distance based topological descriptors.

4. Utility of novel topological descriptors for development of mathematical model for prediction of physicochemical/physical properties like boiling point, cavity surface area, molar refraction etc. for diverse nature of compounds and the comparison with the well-known topological descriptors.

5. Selection of datasets belonging to therapeutic agents of diverse nature with main emphasis on life threatening diseases such as AIDS, cancer, cardiac disorders, neurological disorders, and binding affinities to various receptors.

6. Computation of values of topological descriptors of diverse nature for every analogue in datasets belonging to various categories of therapeutic agents by using an in-house computer program.

7. Analysis of data and identification of active ranges.

8. Development of mathematical models for the prediction of biological activities of various categories of therapeutic agents.


10. Designing of lead structures based upon aforementioned mathematical models and passing on the same to originators for synthesis and biological screening.